Role of Hybridization in the Superconducting Properties of an Extended $d-p$ Hubbard Model: a Detailed Numerical Study

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February 2, 2008

Abstract

The Roth's two-pole approximation has been used by the present authors to study the effects of the hybridization in the superconducting properties of a strongly correlated electron system. The model used is the extended Hubbard model which includes the $d-p$ hybridization, the p-band and a narrow d-band. The present work is an extension of the previous Ref. [3]. Nevertheless, some important correlation functions necessary to estimate the Roth's band shift, are included together with the temperature T and the Coulomb interaction U to describe the superconductivity. The superconducting order parameter of a cuprate system, is obtained following Beenen and Edwards formalism. Here, we investigate in detail the change of the order parameter associated to temperature, Coulomb interaction and Roth's band shift effects on superconductivity. The phase diagram with T_c versus the total occupation numbers n_T, shows the difference respect to the previous work.

PACS numbers: 71.27.+a, 71.10.Fd, 74.25.Dw

The high temperature superconductors discovered by Bednorz and Muller [1] are believed to be explained in the framework of the Hubbard model [2] since electron correlations are strong.

In this work we have used the extended Hubbard model [3] with the Roth's method [4]. In the previous work [3], we improved Ref. [5] to also include superconducting properties following closely the approach introduced by Beenen

and Edwards [6]. Nevertheless, in Ref. [3], the Roth's band shift has been estimated disregarding the temperature and the Coulomb interaction effects. In the present work, we have included these effects in the Roth's band shift. Consequently, due to the U dependence, it is necessary to calculate more correlation functions than in the reference [3]. Therefore, we hope by using this procedure to get a more correct behavior of the superconductor order parameter (as a function of T) and the critical temperature T_c. The Hamiltonian used is:

$$
\begin{aligned}
H \quad = \quad & \sum_{i,\sigma}(\varepsilon_d-\mu)d^{\dagger}_{i\sigma}d_{i\sigma}+\sum_{i,j,\sigma}t^{d}_{ij}d^{\dagger}_{i\sigma}d_{j\sigma}+U\sum_{i}n^{d}_{i\uparrow}n^{d}_{i\downarrow} \\
& +\sum_{i,\sigma}(\varepsilon_p-\mu)p^{\dagger}_{i\sigma}p_{i\sigma}+\sum_{i,j,\sigma}t^{p}_{ij}p^{\dagger}_{i\sigma}p_{j\sigma} \\
& +\sum_{i,j,\sigma}t^{pd}_{ij}\left(d^{\dagger}_{i\sigma}p_{j\sigma+}p^{\dagger}_{i\sigma}d_{j\sigma}\right) \qquad (1)
\end{aligned}
$$

where μ is the chemical potential.

In order to study superconductivity by Roth's method, it is necessary to include "hole" operators in the set of "electron" operators (which describes the normal state) and evaluate anomalous correlation functions. As discussed in Ref. [3], considering the particular case with singlet pairing and the d-wave symmetry, we get $\langle d_{i-\sigma}d_{i\sigma}\rangle=0$ and $\sum_l\langle d_{i-\sigma}d_{l\sigma}\rangle=0$, where the sum is over sites l which are nearest neighbors of i. Therefore, in the d-wave case [6], the superconducting gap is determined by the gap function,

$$
\overline{\gamma}_k \quad = \quad -\overline{\gamma}_k\frac{2n^{d}_{1\sigma}t^{d}U^{2}}{L}\sum_{k}\left[\cos\left(k_xa\right)-\cos\left(k_ya\right)\right]^{2}\frac{1}{2\pi i}\oint f(\omega)G^{13}_{k\sigma}(\omega)d\omega \qquad (2)
$$

where $f(\omega)$ is the Fermi function. The propagators $G^{1s}_{k\sigma}$, with $s=1,2$ or 3 can be obtained as in Ref. [3]. We can readily obtain the correlation function $n^{d}_{1\sigma}=\langle d^{\dagger}_{1\sigma}d_{1\sigma}\rangle$ considering a nearest-neighbor model with $t^{d}_{0j}=t^{d}$ for the z neighbors. In this way it is necessary only one value of $n^{d}_{j\sigma}$, which is $n^{d}_{1\sigma}$. The gap function given by equation (2), defined in Ref. [6], is solved self-consistently. The band shift $W_{k\sigma}=W^{d}_{k\sigma}+W^{pd}_{\sigma}$, shifts the poles of the propagators $G^{1s}_{k\sigma}$. In this work we considered a k independent hybridization $(V^{pd}_{0})^{2}=\langle V^{dp}_{k}V^{pd}_{k}\rangle$ as discussed in Ref. [5], where $\langle ...\rangle$ is the average over the Brillouin zone and $V^{dp}_{k}(V^{pd}_{k})$ are the Fourier transform of $t^{dp}_{ij}(t^{pd}_{ij})$. Consequently, the W^{pd}_{σ} term is k independent, and also, its temperature and Coulomb interaction dependence is quite small. Thus, our focus here is $W^{d}_{k\sigma}$ which is given by:

$$
\begin{aligned}
W^{d}_{k\sigma} \quad = \quad & -\frac{1}{n^{d}_{\sigma}(1-n^{d}_{\sigma})}\sum_{j\neq 0}t^{d}_{0j}\left\{(n^{d}_{j\sigma}-2m_{j\sigma})+e^{i\mathbf{k}\cdot\mathbf{R}_j}\left[\frac{\alpha_{j\sigma}n^{d}_{j\sigma}+\beta_{j\sigma}m_{j\sigma}}{1-\beta_{\sigma}\beta_{-\sigma}}\right.\right. \\
& \left.\left.+\frac{\alpha_{j\sigma}n^{d}_{j-\sigma}+\beta_{j\sigma}m_{j-\sigma}}{1+\beta_{\sigma}}+\frac{\alpha_{j\sigma}n^{d}_{j-\sigma}+\beta_{j\sigma}(n^{d}_{j-\sigma}-m_{j-\sigma})}{1-\beta_{\sigma}}\right]\right\} \qquad (3)
\end{aligned}
$$

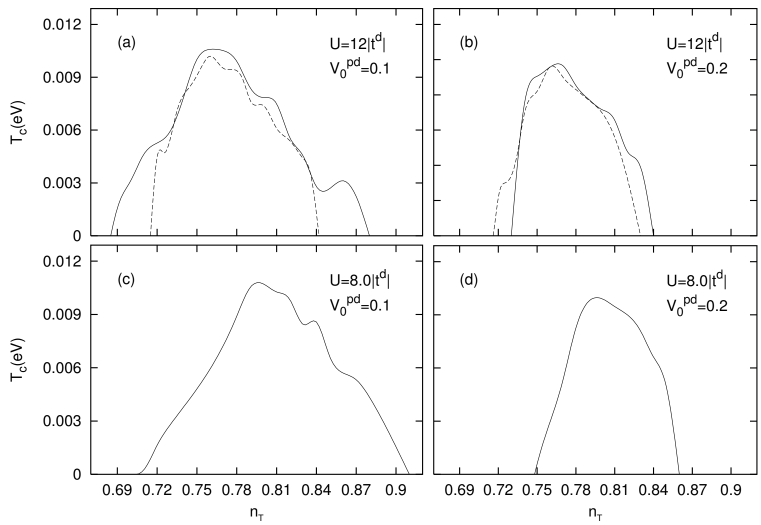

Figure 1: T_c as a function of the total occupation number n_T (where $n_T = n^d_\sigma + n^d_{-\sigma}$). In (a) and (b), the dotted lines show the previous results from Ref. [3] for $U = 12|t^d|$. The solid lines show the behavior of T_c in the present approach. The figures (c) and (d) show the present results for $U = 8|t^d|$. The units of the hybridization V_0^{pd} are electron-volts (eV). ($t^d = -0.5eV$.)

where α and β are defined as:

$$\alpha_{j\sigma} = \frac{n^d_{j\sigma} - m_{j\sigma}}{1 - n^d_{-\sigma}} \quad \text{and} \quad \beta_{j\sigma} = \frac{m_{j\sigma} - n^d_{-\sigma} n^d_{j\sigma}}{n^d_{-\sigma}(1 - n^d_{-\sigma})}, \tag{4}$$

with $n^d_{-\sigma} \equiv n^d_{0-\sigma}$. The correlation function $m_{j\sigma} = \langle d^\dagger_{0\sigma} n^d_{j-\sigma} d_{j\sigma} \rangle$ is obtained from the propagator $G^{12}_{k\sigma}$ (see Ref. [3]) as:

$$m_{j\sigma} = \frac{1}{2\pi i} \oint f(\omega) \frac{1}{L} \sum_k e^{i\mathbf{k}\cdot\mathbf{R}_j} G^{12}_{k\sigma}(\omega) d\omega. \tag{5}$$

The band shift given by equation (3) can be split into a **k**-dependent and a **k**-independent term. While the role of the **k**-independent term is only to shift the poles of the Green's function, the **k**-dependent part causes a flattening at the top of the lower band from around $\mathbf{k} = (\pi, \pi)$ until $\mathbf{k} = (\pi, 0)$ as can be verified in Refs. [6, 8]. This flattening occurs because $W^d_{k\sigma}$ decreases when ε^d_k increases, as discussed in Ref. [6]. This numerical calculations agree with the Monte Carlo results obtained by Bulut *et al* [6, 8]. The flattening in the quasi-particle sub-bands (called Hubbard bands) leads to a band narrowing of

these sub-bands, increasing the gap originated by the Coulomb interaction U. Our numerical results show that the *narrowing* of the sub-bands decreases with increasing U. This fact is very important, because this leads to a change at the position of the chemical potential μ which is relevant to obtain the behavior of the high-temperature superconductivity [8]. In the figures 1(a)-1(b) are shown phase diagrams with the dotted lines corresponding to the results obtained in Ref. [3], where the effects of the temperature T and the Coulomb interaction are not included in $W_{k\sigma}$. In the figures 1(c)-1(d) the value of the U is decreased. The solid lines show the results for T_c, with the effects of T and U included in the calculation of the $W^d_{k\sigma}$ band shift. The results show a small increase of T_c when we consider in $W^d_{k\sigma}$ the effects of T and U. We believe that the increasing of T_c occurs as result of the change in the value of the chemical potential, as discussed above. The numerical results show also that in the interval of temperatures showed in figure 1 the effect of the temperature in $W^d_{k\sigma}$ is quite small.

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